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Theoretical Predictions of Phase Transitions at Ultra-high Pressures

BRIAN BOATES, Dalhousie University, Lawrence Livermore National Laboratory

We present ab initio calculations of the high-pressure phase diagrams of important planetary materials such as CO2, MgSiO3, and MgO. For CO2, we predict a series of distinct liquid phases over a wide pressure (P) and temperature (T) range, including a first-order transition to a dense polymer liquid. We have computed finite-temperature free energies of liquid and solid CO2 phases to determine the melting curve beyond existing measurements and investigate possible phase separation transitions. The interaction of these phase boundaries with the mantle geotherm will also be discussed. Furthermore, we find evidence for a vast pressure-temperature regime where molten MgSiO3 decomposes into liquid SiO2 and solid MgO, with a volume change of approximately 1.2 percent. The demixing transition is driven by the crystallization of MgO ? the reaction only occurs below the high-pressure MgO melting curve. The predicted transition pressure at 10,000 K is in close proximity to an anomaly reported in recent laser-driven shock experiments of MgSiO3. We also present new results for the high-pressure melting curve of MgO and its B1-B2 solid phase transition, with a triple point near 364 GPa and 12,000 K.